

Forget those \$%@*!?!& commands: The Practical Supercomputing Toolkit

<http://www.pstoolkit.org>

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... and the users who have provided valuable feedback



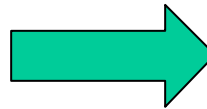
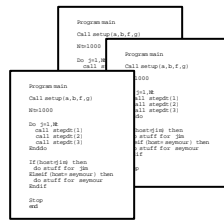
DoD UGC, June 2001, Biloxi



CoRA, NWRA, Inc.

The Problem

The Problem



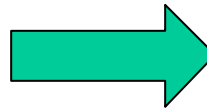
The Problem

Code A

```

Program main
    Call setenv(a,b,f,g)
Mio1000
Do 101-100
    Program main
        Call setenv(a,b,f,g)
    1000
Program main
    Call setenv(a,b,f,g)
Mio1000
Do 101-100
    call setenv(1)
    call setenv(2)
    call setenv(3)
    Break
If (testenv) then
do until f for 3m
Call Setenv(setenv) then
do until f for anyother
if
Stop
end

```



Cite A

Code B

```

Program main
  Call setup(a,b,f,g)
  Mv1000
  Do 30-100
    Call setup(a,b,f,g)
  End1000

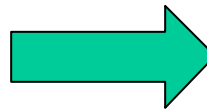
Program main
  Mv1000
  Do 30-100
    Call setup(a,b,f,g)
  End1000

Program main
  Mv1000
  Do 30-100
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  End1000

  If (count=0) then
    do stuff for 3m
  Else (stuff anymore) then
    do stuff for anymore
  EndIf

  stop
end

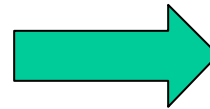
```



Cite B

The Problem

Code A

[illegible]

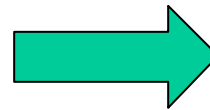
Cite A

Code B

[illegible]

Cite B

Code C

[illegible]

Cite C

The Problem

host	mkdir	put/get	migrate	queue
ERDC/jim	msfmkdir	msfput, msfget msfmput, msfmget	msfdmput, msfdmget	PBS
NAVO/seymour	remsh jules mkdir remsh vincent mkdir	rcp \$f jules-hip0:\$d rcp \$f vincent-hip0:\$d	remsh jules release remsh vincent release	NQS
ASC/hpc03-1	mkdir	/usr/bsd/rcp \$f \$(msas):\$ARC/\$d		PBS
AHPCRC/md	mkdir	cp	dmpu t, dmget	NQS
PSC/jaromir	far mkdir	far store far get		NQS
SDSC/golden	pftp mkdir hsi mkdir	pftp cd \$d, put pftp cd \$d, get		NQS
UCAR/ouray	****	mswrite, msread	-offline	NQS

The Problem

- Unnecessary spin up time for new users,
- Dependence on specific sites/hardware,
- Reduced productivity,
- Increased project cost,
- Discouraged users,
- Duplicated effort.

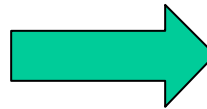
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    Break
If (testenv) then
do until f for 3m
Call Setenv(setenv) then
do until f for anyother
if
Stop
end

```



Cite A

Code B

```

Program main
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  Do 30-100
    Call setup(a,b,f,g)
  End1000

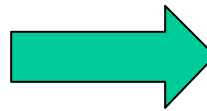
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  If (count=0) then
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  EndIf

  stop
end

```



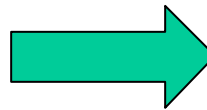
Cite B

Code C

```

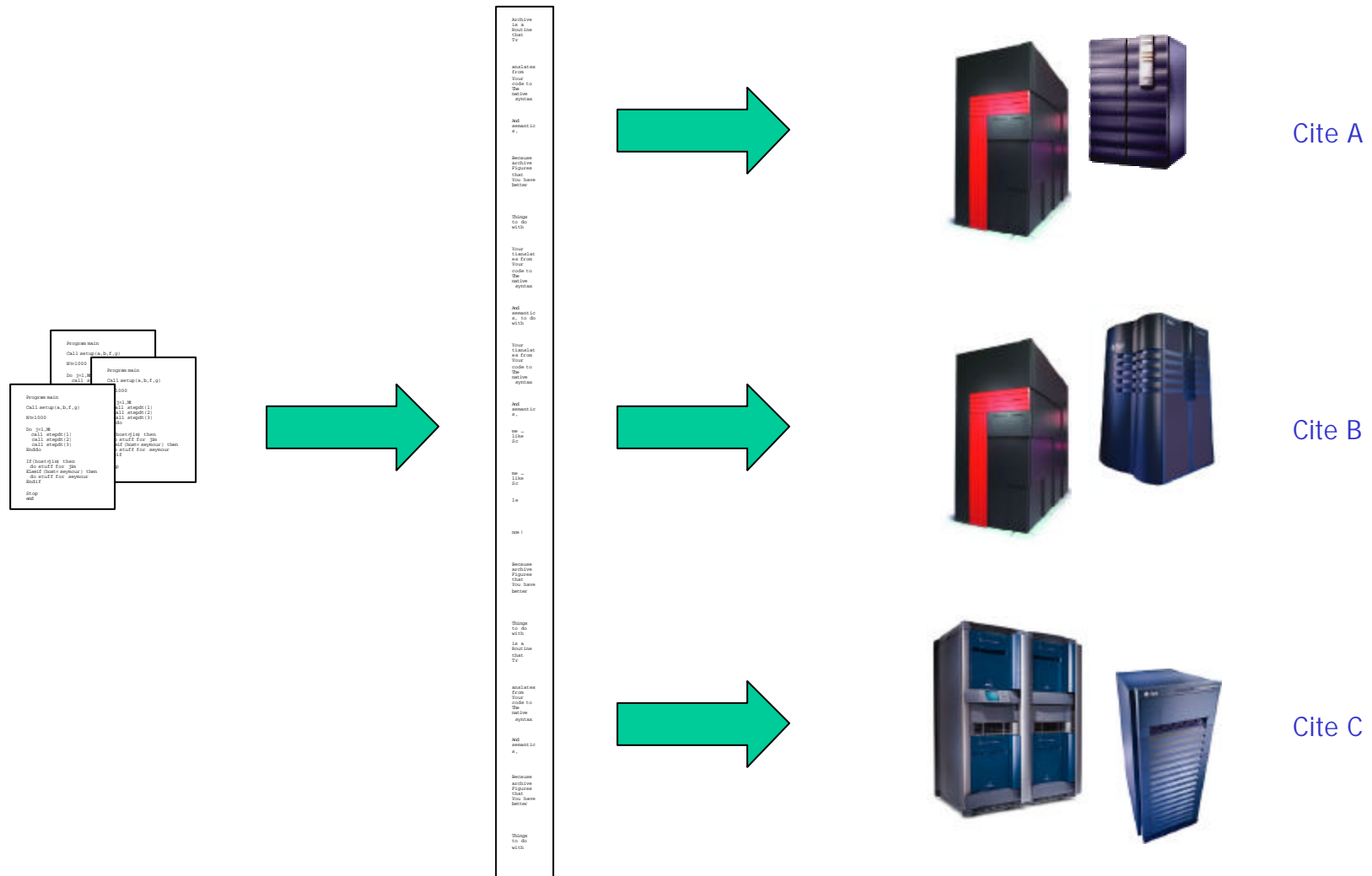
Program main
  Call seqproc(B,F,g)
Writeln
Program main
  Do 3 to 100
    Call seqproc(A,B,f,g)
  Writeln
Program main
  Do 3 to 100
    Call seqproc(A,B,f,g)
  Writeln
  Do 3 to 100
    call seqproc(1)
    call seqproc(2)
    call seqproc(3)
  Writeln
  If (count=0) then
    write('for 3m')
  else if (count>0) then
    write('there are',count,'
    3m')
  Writeln
  If (count=0) then
    do until for 3m
      count:=count+1
    until for 3m
  Writeln
  If (count=0) then
    do until for 3m
      count:=count+1
    until for 3m
  Writeln
  Stop
end

```



Cite C

The Solution



HPCMO & Metacomputing Working Group Initiative

Goals:

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- Provide translation tools to all DoD users in the form of a uniform command-line interface.

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- Write nimble translation tools that are modular, maintainable, and reusable.

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Goals:

- Provide translation tools to all DoD users in the form of a uniform command-line interface.
- Write nimble translation tools that are modular, maintainable, and reusable.
- Shepherd implementation on all major U.S. super-computer centers – not just the DoD centers.

The Solution

How many translation tools do you need?

The Solution

How many translation tools do you need?

2

qprep, archive

The Solution

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2

qprep, archive

Unless you can think of more.

But can you?

The Solution

Tools for Uniform SuperComputing (TUSC): `qprep`



`qprep`:

simplifies and unifies job submission to queues

`qprep` is not a replacement for existing queuing systems, e.g., PBS, NQS, ...

rather, `qprep` is a translator between them.

The Solution

Tools for Uniform SuperComputing (TUSC): qprep

qprep is planned to work in two ways, both of which are intended to be familiar to users:

1. Command-line arguments:

```
qprep script -mpp_p 512 -mpp_t 12.45 ...
```

2. Pseudo-comment directives in script preamble:

```
#PSTQ -l mpp_p 512  
#PSTQ -l mpp_t 12.45  
...
```

qprep will edit the script, translating the preamble to the native queuing system.

The Solution

Tools for Uniform SuperComputing (TUSC): qprep

The current plan is for implementation to be as simple as filling out a “translation table”.

Prototype code for `qprep` is currently running on the T3E's at ERDC, NAVO, and AHPCRC, and on the Origin 2000 machines at ASC.

The Solution

Tools for Uniform SuperComputing (TUSC): archive



archive:

simplifies and unifies using data archives

`archive` provides a collection of commands to manipulate archival data, including `put`, `get`, `ls`, `stat`, `mkdir`, each of which accepts a list of command-line options.

Current plans include implementation of `mv`, `rm`, `rmdir`, `chmod`, `chgrp`, and `chown` as well.

The Solution

Tools for Uniform SuperComputing (TUSC): archive

archive is written in two layers:

- `archive.pm` is a Perl module containing subroutines that are site-independent.
- `local.pm` is a Perl module which contains subroutines that depend on the local system.

`local.pm` intentionally contains as little code as possible and ample comment statements to facilitate implementation at a new site.

The Solution

Tools for Uniform SuperComputing (TUSC): [archive](#)

Prototype code for [archive](#) is currently running on the T3E's at ERDC, NAVO, And AHPCRC, and on the Origin 2000 machines at ASC.

The following POC's for implementation, maintenance, and improvement of [archive](#) and [qprep](#) have been assembled: [Steve Thompson](#) (ARL), [Bill Asbury](#), [Anthony DelSorbo](#) (ASC), [Virginia Bedford](#) (ARSC), [Bradford Blasing](#) (AHPCRC), [Rebecca Fahey](#), [David Sanders](#) (ERDC), [Mitch Murphy](#) (MHPCC), [John Skinner](#) (NAVO), [Mark Dotson](#), and [Winfried Bernhard](#) (WPAFB).

The Practical Supercomputing Toolkit



To facilitate implementation and distribution of the DoD uniform command-line interface, including [archive](#) and [qprep](#) ...

the HPCMO has funded the development of the [Practical Supercomputing Toolkit \(PST\)](#).

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- Freely available from www.pstoolkit.org.

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- Open source, allowing users to contribute their own solutions to problems for the good of the user community, and in turn benefit from the solutions of others.
- Freely available from www.pstoolkit.org.
- Written primarily in Perl so as to benefit from Perl's advanced text processing capability, vast user support, and its Plain Old Documentation (POD) system. With POD, source code comments can be easily used to generate documentation as [man pages](#), [HTML](#), [LaTeX](#), or [Framemaker](#).

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- Soliciting users for input on requirements for tools.

The PST Layers

TUSC (Tools for Uniform Supercomputing)

Translation tools (including [qprep](#) and [archive](#)) that hide site-specific details.

SET (Source Editing Tools)

Tools that simplify the process of preparing source code for execution.

MD (Maintenance and Documentation)

Routines to install, update, and document PST.

ACT (Application Cookbook Tools)

A repository of problem-specific samples and tutorials built with TUSC and SET. A collection of contributions by veteran users that gathers and disseminates experience.

Netscape: Practical Supercomputing Toolkit

File Edit View Go Communicator Help

Back Forward Reload Home Search Netscape Print Security Shop Stop

Bookmarks Location: <http://www.pstoolkit.org/> What's Related

Internet Lookup New&Cool

PST

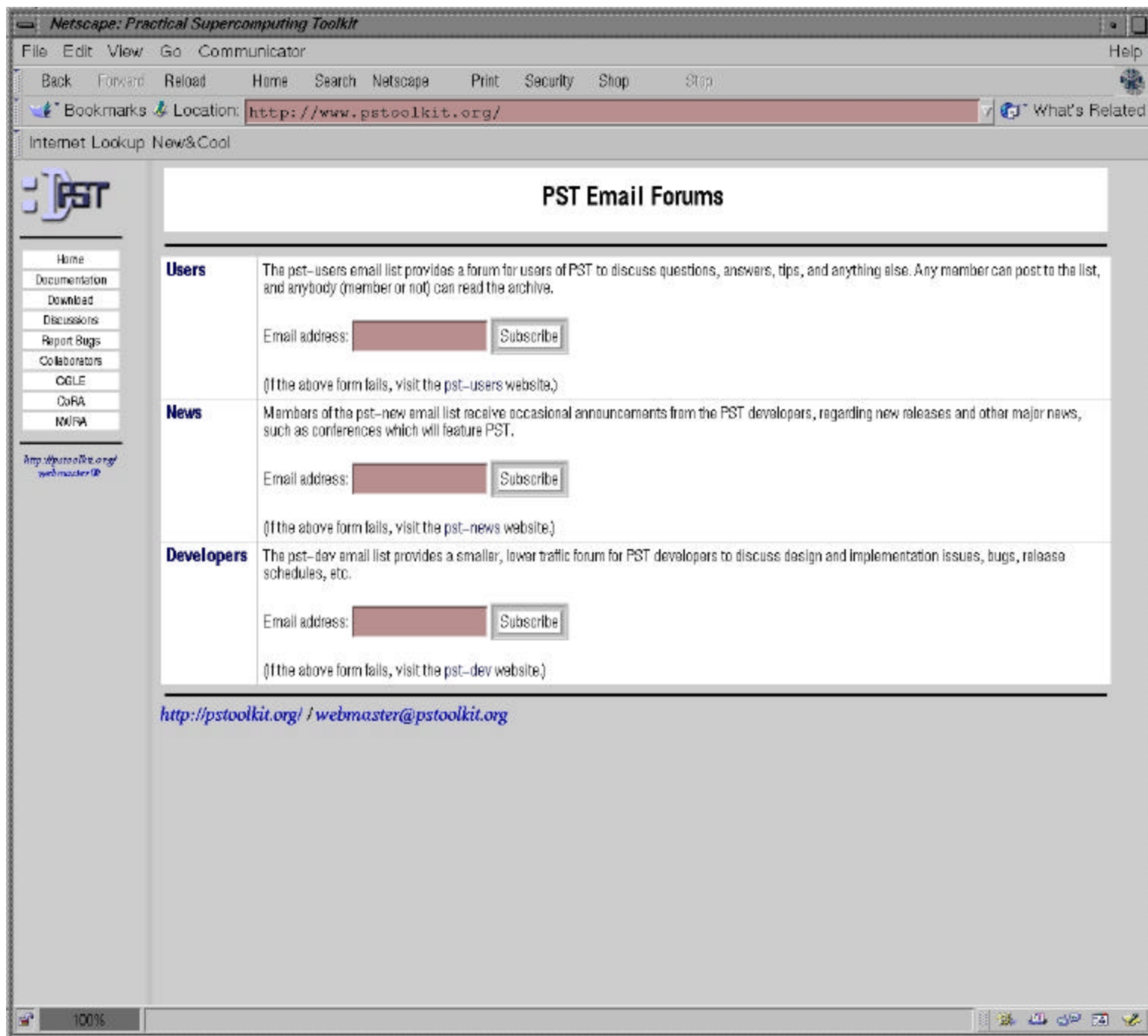
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<http://pstoolkit.org/>
webmaster@

Practical Supercomputing Toolkit

Problem	Most major supercomputer centers, including those operated by the the Department of Defense (DoD) High Performance Computing Modernization Program (HPCMP) and the National Science Foundation (NSF), provide critical resources and services to the user community. Nevertheless, because of disparate hardware and software systems at individual supercomputer sites, users must learn myriad center-specific software syntax and semantics to perform even the most mundane operations, such as archival data storage and job submission. Furthermore, as users pursue the larger and more complex computer simulations possible with advancing supercomputer hardware, batch job scripts and code become more complicated, and the user's need to maintain portable, site-independent routines is intensified. The fact that most users are trained in mathematical, physical, or engineering disciplines, rather than computer science or software system development, only compounds this problem.										
Objective	The Practical Supercomputing Toolkit intends to mitigate problems associated with non-expert users making use of supercomputing facilities.										
Methods	<p>PST provides or will provide:</p> <ul style="list-style-type: none"> • a software system built from stand-alone layers which can be used as a full suite of routines or as a truncated system comprised of a subset of layers; • open source policy to encourage development participation from users and client site administrators; • unified internal/external documentation to simultaneously enhance usability and modifiability of source code; <p>Planned software layers include:</p> <ul style="list-style-type: none"> • TUSC (Tools for Unification of SuperComputing): standards and utilities for a unified command-line interface for archive and job queue submission at all major U.S. supercomputer centers and other supported sites; • SET (Source Editing Tools): routines to automate, simplify, and unify the process of preparing source code for execution; • MD (Management and Documentation): suite of routines to install, update, maintain, and document the PST software; • ACT (Application Cookbook Tools): a repository of problem- and user-specific sample code and tutorials to disseminate the experience of veteran users; 										
Timeline	<table border="1"> <thead> <tr> <th>Date</th> <th>Goal</th> </tr> </thead> <tbody> <tr> <td>2001 May</td> <td>Alpha release of PST to DoD Shared Resource Centers: <ul style="list-style-type: none"> • "archive" syntax specification, • "archive" front end, • "archive" documentation, • "archive" sample back end for one MSRC, • Web site, • FTP site, • Email forums. </td> </tr> <tr> <td>2001 June 8</td> <td>Advertise PST to DoD Shared Resource Centers.</td> </tr> <tr> <td>2001 June 18-21</td> <td>Announcement of PST to DoD HPC UGC in Biloxi, Mississippi</td> </tr> <tr> <td>2001 July 15-18</td> <td>Presentation at the Second Global Grid Forum (GGF-2) in Vienna, Virginia</td> </tr> </tbody> </table>	Date	Goal	2001 May	Alpha release of PST to DoD Shared Resource Centers: <ul style="list-style-type: none"> • "archive" syntax specification, • "archive" front end, • "archive" documentation, • "archive" sample back end for one MSRC, • Web site, • FTP site, • Email forums. 	2001 June 8	Advertise PST to DoD Shared Resource Centers.	2001 June 18-21	Announcement of PST to DoD HPC UGC in Biloxi, Mississippi	2001 July 15-18	Presentation at the Second Global Grid Forum (GGF-2) in Vienna, Virginia
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100%



The Future of PST

Over the next 18 months, tools will be implemented, released, and refined based on user input, and the number of centers that support **PST** will increase, aided by the open source philosophy.

July 15, 2001

Initial release of **qprep** man page.

December, 2001

qprep version 1.0 release.

May, 2002

Initial release of **MD** and **SET** layers.

October, 2002

Full release of **TUSC**, **MD**, and **SET** layers.

ACT layer codes will be released as contributed by users.

You can impact the development of PST

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- The evolution of **PST** relies on users for feedback on tool definition and implementation, as well as code submissions from user/developers.

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- Because [PST](#) is open source, developers at other centers can contribute implementations of [archive](#), which will then be added to the full distribution.

Acknowledgments

The DoD High Performance Computing Modernization Office provides the initial funding of the TUSC, SET, and MD layers of PST, with emphasis on unification across DoD Shared Resource Centers for job submission and data archiving processes. The DoD Metacomputing Working Group provides logistical coordination to encourage the participation of the DoD centers.